数理解析研究所講究録
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Notes on effective usage of double exponential formulas for numerical integration.

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## 1. Introduction

We shall describe the results of numerical evaluation of an integral

(1-1) $$I = \int_a^b f(x)\,dx$$

using the double exponential formulas (DE formulas), and empirical evidences derived from these results.

The DE formulas have been developed as a class of numerical quadrature formulas by Takahashi and Mori [1], and they offer one of the most powerful methods to evaluate an improper integral on $[a,b]$, in which the integrand is singular at one endpoint or both. Moreover, we shall show a method to evaluate difficult integrals, where the integrand is highly oscillating.

## 2. Comparison of results by some numerical integration formulas.

As a numerical comparison of formulas among DE, IMT, CADRE and QUAD we show in Table 2-1 the number of integrand evaluations and the relative error estimated from the following convergence criterion (2-1) by choosing 15 test cases of Patterson [3] and Ichida and Kiyono [4].

A convergence criterion of our program is satisfied when

(2-1) $$|S_{i+1} - S_i| \leq \varepsilon |S_{i+1}|$$

where $S_i$ is a value of DE formula with mesh size $h_i$, and $S_{i+1}$ is a value of DE formula with mesh size $h_{i+1} = h_i/2$, and $\varepsilon$ is some preassigned tolerance (e.g., $10^{-9}$).

## 2.1 DE formula and IMT formula

Table 2.1-1

| DE | IMT |
|---|---|
| $I = \int_a^b f(x)\,dx$<br>$x = \phi(u)^*$<br><br>$I = \int_{-\infty}^{\infty} f(\phi(u))\,\phi'(u)\,du$<br>$\approx I_h = h\sum_{n=-\infty}^{\infty} f(\phi(nh))\,\phi'(nh)$<br>based on the fact that the trapezoidal rule gives the best result for $\int_{-\infty}^{\infty} g(u)du$ with mesh size $h$ . | $I = \int_0^1 f(x)\,dx$<br>$x = \psi(u) = \frac{1}{Q}\int_0^u \exp(-\frac{1}{t} - \frac{1}{1-t})\,dt$<br>$Q = \int_0^1 \exp(-\frac{1}{t} - \frac{1}{t-1})\,dt$<br>$I = \int_0^1 f(\psi(u))\,\psi'(u)\,du$<br>$\approx S_n = \frac{1}{N}\sum_{n=1}^{N-1} f(\psi(\frac{n}{N}))\,\psi'(\frac{n}{N})$<br>based on Euler-Maclaurin summation formula. |

* where

(2.1-1) $\quad x = \phi(u) = \tanh(\frac{\pi}{2}\sinh u) \quad$ if $\quad I = \int_{-1}^{1} f(x)\,dx$

(2.1-2) $\quad x = \phi(u) = \exp(\frac{\pi}{2}\sinh u) \quad$ if $\quad I = \int_0^{\infty} f(x)\,dx$

(2.1-3) $\quad x = \phi(u) = \exp(u - \exp(-u)) \quad$ if $\quad I = \int_0^{\infty} \exp(-x)\,f(x)\,dx$

(2.1-4) $\quad x = \phi(u) = \sinh(\frac{\pi}{2}\sinh u) \quad$ if $\quad I = \int_{-\infty}^{\infty} f(x)\,dx$

Table 2-1 Comparison of results by DE, IMT, CADRE and QUAD

| | D E | IMT | CADRE | QUAD |
|---|---|---|---|---|
| $P_1$ $\int_0^1 \sqrt{x}\, dx = \frac{2}{3}$ | 44 $3.3_{10}{-12}$ | 127 $4.9_{10}{-13}$ | 129 $1.2_{10}{-10}^*$ | 361 $2.2_{10}{-10}^*$ |
| $P_2$ $\int_{-1}^1 (0.92 \cosh x - \cos x)\, dx = 1.84 \sinh 1 - 2 \sin 1$ | 96 $1.7_{10}{-12}$ | 127 $2.4_{10}{-12}$ | 33 $1.3_{10}{-13}^*$ | 37 $2.1_{10}{-14}^*$ |
| $P_3$ $\int_{-1}^1 \frac{dx}{x^4 + x^2 + 0.9} \doteqdot 1.5822\ 32964$ | 92 $3.1_{10}{-11}$ | 127 $2.8_{10}{-13}$ | 129 $4.2_{10}{-12}^*$ | 73 $1.5_{10}{-12}^*$ |
| $P_4$ $\int_0^1 x^{\frac{3}{2}}\, dx = \frac{2}{5}$ | 40 $1.0_{10}{-11}$ | 127 $8.1_{10}{-13}$ | 529 $2.7_{10}{-10}^*$ | 163 $5.0_{10}{-12}^*$ |
| $P_5$ $\int_0^1 \frac{dx}{1 + x^4} = \frac{1}{4\sqrt{2}}\left\{\log(3 + 2\sqrt{2}) + \pi\right\}$ | 92 $2.3_{10}{-12}$ | 127 $5.6_{10}{-13}$ | 65 $2.1_{10}{-10}^*$ | 73 $0^*$ |
| $P_6$ $\int_0^1 \frac{dx}{2 + \sin 10\pi x} = \frac{2}{\sqrt{3}}$ | 724 $1.2_{10}{-10}$ | 509 $2.2_{10}{-12}$ | 785 $8.4_{10}{-12}^*$ | 757 $3.3_{10}{-13}^*$ |

| | | | | |
|---|---|---|---|---|
| $P_7$ $\int_0^1 \frac{x}{e^x - 1} dx \doteqdot 0.77750\ 46341$ | 48 $3.4_{10}-12$ | 127 $6.6_{10}-13$ | 17 $2.2_{10}-12^*$ | 37 $2.1_{10}-14^*$ |
| $P_8$ $\int_{0.1}^1 \frac{\sin 100\pi x}{\pi x} dx$ | 620 $2.5_{10}-13$ | 509 $4.1_{10}-16$ | 3505 $3.2_{10}-12^*$ | 2773 $5.6_{10}-13^*$ |
| $P_9$ $\int_0^{10} \frac{50}{\pi(2500 x^2 + 1)} dx = \frac{1}{\pi} \tan^{-1} 500$ | 180 $2.2_{10}-10$ | 255 $1.5_{10}-11$ | 337 $1.3_{10}-11^*$ | 343 $3.3_{10}-12^*$ |
| $P_{10}$ $\int_0^{\pi} \cos(\cos x + 3 \sin x + 2 \cos 2x + 3 \sin 2x + 3 \cos 3x)\, dx$ | 186 $8.6_{10}-12$ | 127 $1.2_{10}-12$ | 417 $1.5\ -12^*$ | 343 $1.0_{10}-12^*$ |
| $P_{11}$ $\int_0^1 \log x\, dx = -1$ | 44 $3.9_{10}-13$ | 127 $2.0_{10}-11$ | 369 $4.5\ -9^*$ | 415 $5.7_{10}-7^*$ |

The results with superscript * are due to Ninomiya's paper.

| | | | | | |
|---|---|---|---|---|---|
| $K_1$ $\int_{-1}^{1} \frac{2^{-\alpha}}{4^{-\alpha} + x^2}\, dx$ | $\alpha = 1$ | 202 $2.4_{10}{-13}$ | 127 $2.3_{10}{-13}$ | 49 $1.2_{10}{-7}^{**}$ | 63 $1.6_{10}{-8}^{**}$ |
| $= 2 \tan^{-1} 2^{\alpha}$ | $K_1'$ | 103 $1.7_{10}{-14}$ | 127 $7.0_{10}{-13}$ | | |
| $\alpha = 1, 2, \ldots, 31$ | $\alpha = 8$ | 24450 $2.5_{10}{-12}$ | ............ | 1440 $3.4_{10}{-8}^{**}$ | 567 $3.0_{10}{-8}^{**}$ |
| | $K_1'$ | 204 $2.0_{10}{-12}$ | 255 $2.3_{10}{-13}$ | | |
| $\left( K_1' \quad 2\int_{0}^{1} \frac{2^{-\alpha}}{4^{-\alpha} + x^2}\, dx \right)$ | $\alpha = 31$ | ............ | ............ | ........... | ........... |
| | $K_1'$ | 786 $5.9_{10}{-12}$ | 509 $5.4_{10}{-3}$ | | |
| $K_2$ $\int_{0}^{1} x^{\alpha}\, dx = \frac{1}{\alpha + 1}$ | $\alpha = -.1$ | 53 $2.1_{10}{-14}$ | 127 $4.5_{10}{-12}$ | 2452 $1.0_{10}{-7}^{**}$ | 357 $1.4_{10}{-6}^{**}$ |
| | $K_1'$ | 89 $7.3_{10}{-10}$ | | | |
| $\alpha = -.1, -.2, \ldots, -.9, -.99$ | $\alpha = -.8$ | 64 $7.3_{10}{-16}$ | 509 $5.3_{10}{-10}$ | 3043 $2.1_{10}{-6}^{**}$ | 3297 $4.7_{10}{-6}^{**}$ |
| | $K_2'$ | 185 $1.4_{10}{-13}$ | | | |
| $\left( K_2' \quad \int_{0}^{\infty} e^{-(1+\alpha)x} dx \right)$ | $\alpha = -.9$ | 2013 $6.2_{10}{-10}$ | 509 $1.7_{10}{-7}$ | 3532 $9.5_{10}{-2}^{**}$ | 6699 $1.2_{10}{-4}^{**}$ |
| | $K_2'$ | 189 $4.8_{10}{-12}$ | | | |
| | $\alpha = -.99$ | ............ | | | |
| | $K_2'$ | 394 $2.1_{10}{-16}$ | | | |
| $H_1$ $\int_{0}^{1} \log\lvert\log x\rvert\, dx = -\gamma$ | | 48 $2.2_{10}{-11}$ | 121 $3.1_{10}{-11}$ | | |

The results with superscript ** are due to Ichida and Kiyono [4] , $\varepsilon = 10^{-7}$

P6

$$f(x) = \frac{2}{2 + \sin 10\pi x}$$

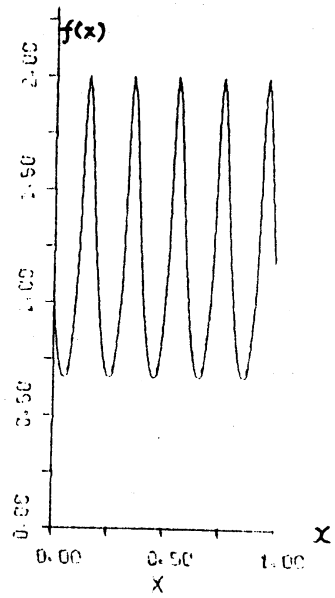



Figure 2-1

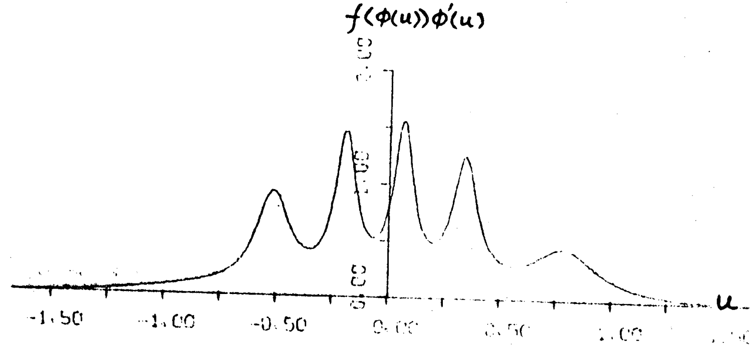



Figure 2-2

P7

$$f(x) = \frac{x}{e^{x} - 1}$$

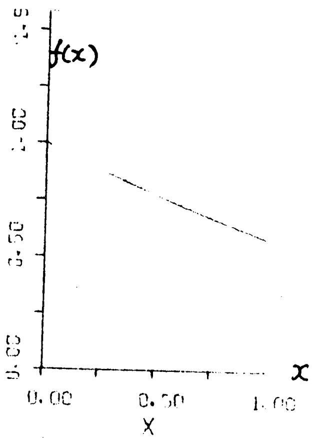



Figure 2-3

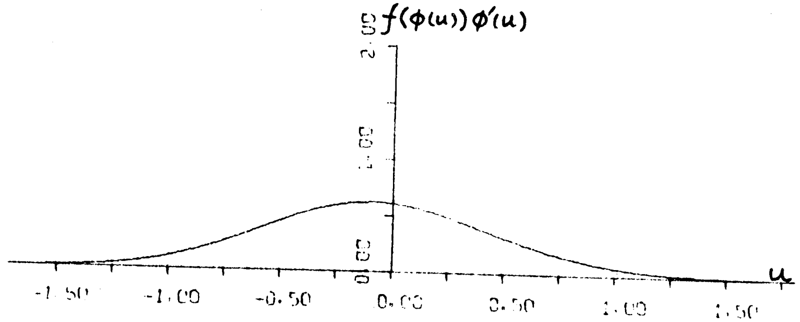



Figure 2-4

P 8

$$f(x) = \frac{\sin 100\pi x}{\pi x}$$

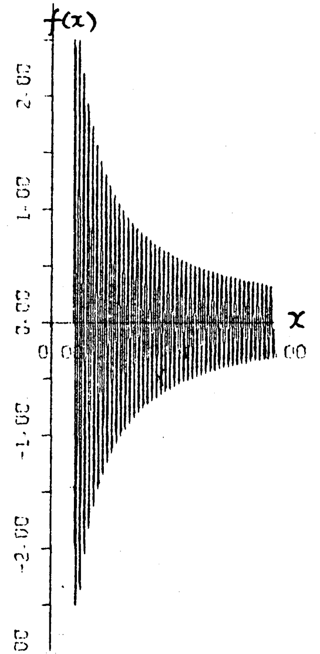



Figure 2-5

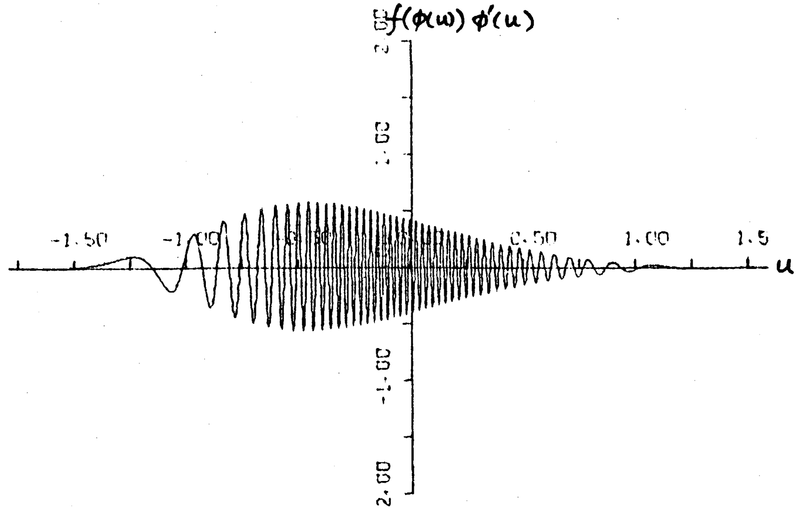



Figure 2-6

P 10

$$f(x) = \cos(\cos x + 3\sin x + 2\cos 2x + 3\sin 2x + 3\cos 3x)$$

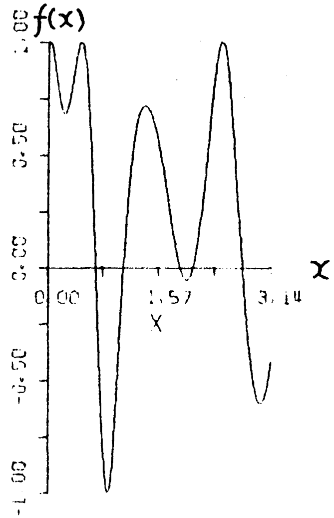



Figure 2-7

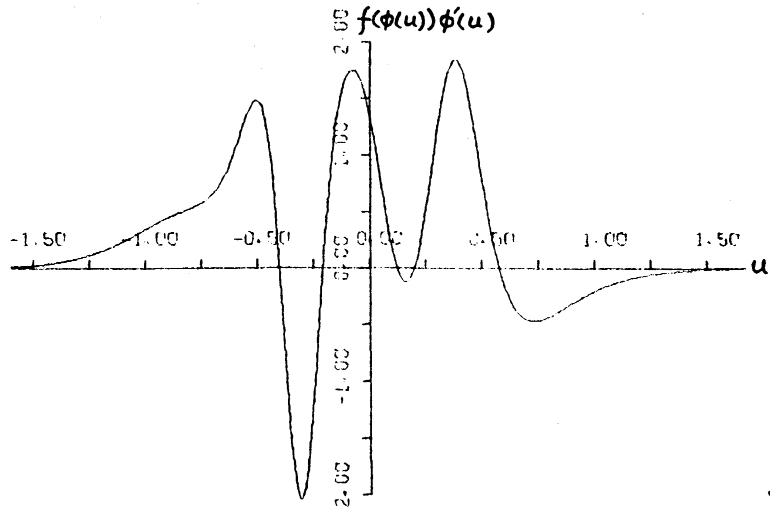



Figure 2-8

K 1

$$f(x) = \frac{2^{-\alpha}}{4^{-\alpha} + x^2}$$

$\alpha = 2, 4, 6, 8, 10$

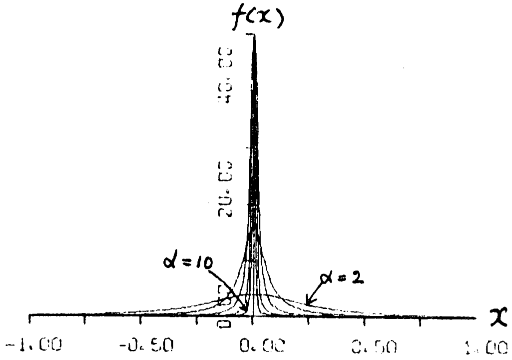



Figure 2-9

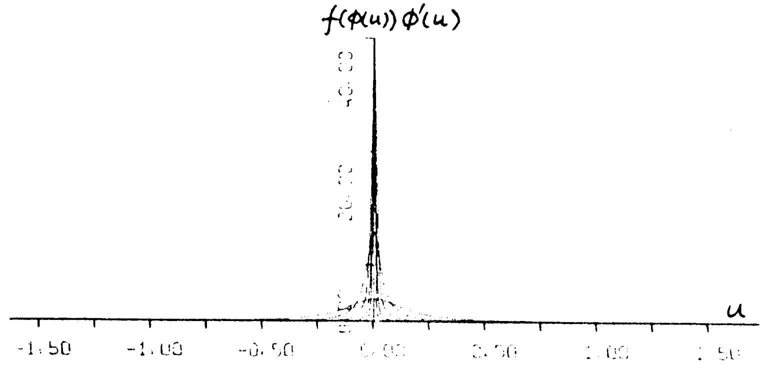



Figure 2-10-1

K 1'

$$\int_{-1}^{1} f(x)\,dx = 2\int_{0}^{1} f(x)\,dx = \int_{-1}^{1} f\left(\frac{x+1}{2}\right) dx$$

$$= \int_{-1}^{1} g(x)\,dx$$

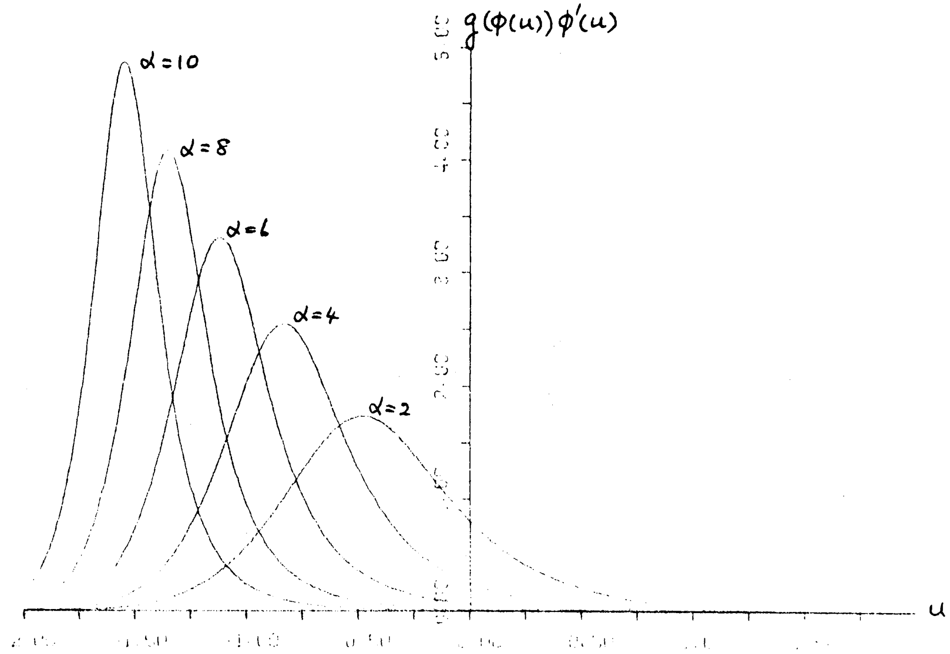



Figure 2-10-2

K 2

$f(x) = x^{\alpha}$ ,  $\alpha = -0.1$ , $-0.9$

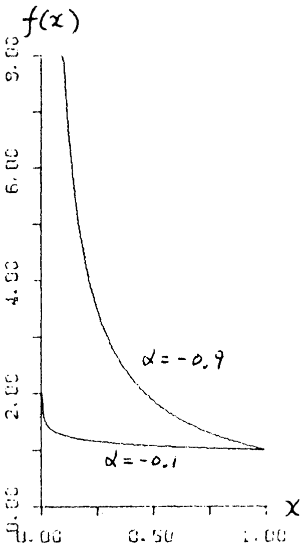



Figure 2-11

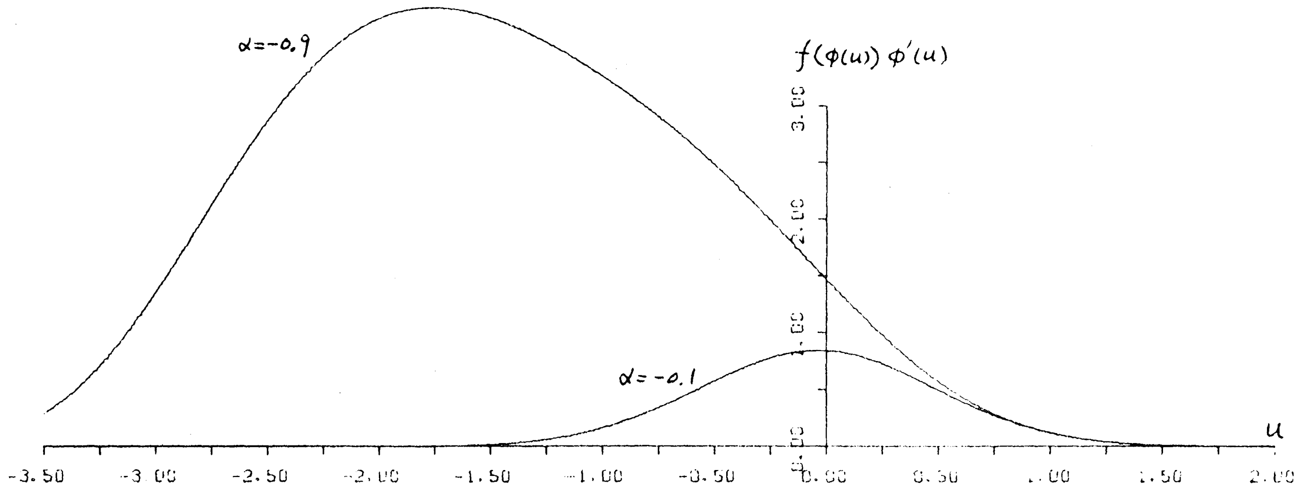



Figure 2-12

H 1

$f(x) = \log|\log x|$

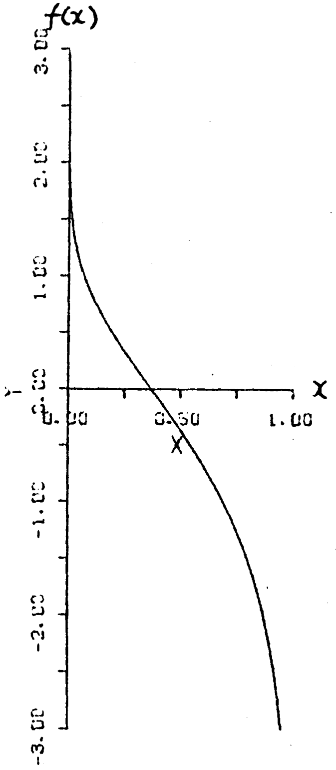



Figure 2-13

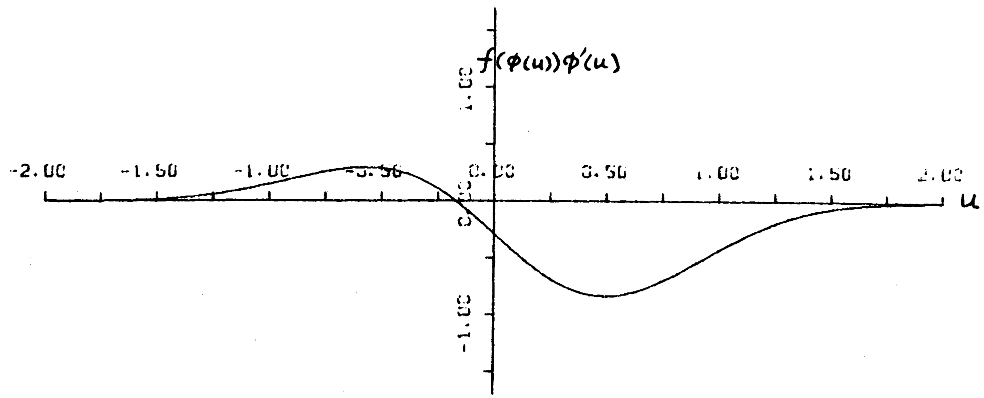



Figure 2-14-1

IMT quadrature

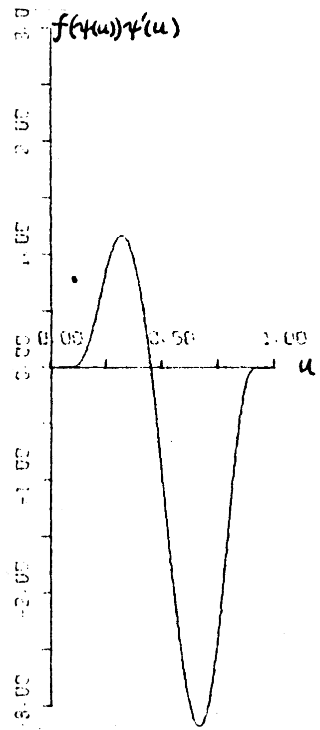



Figure 2-14-2

H1′

$$\int_0^1 \log|\log x|\,dx = \int_0^\infty e^{-x}\log x\,dx = \int_0^\infty f(x)\,dx$$

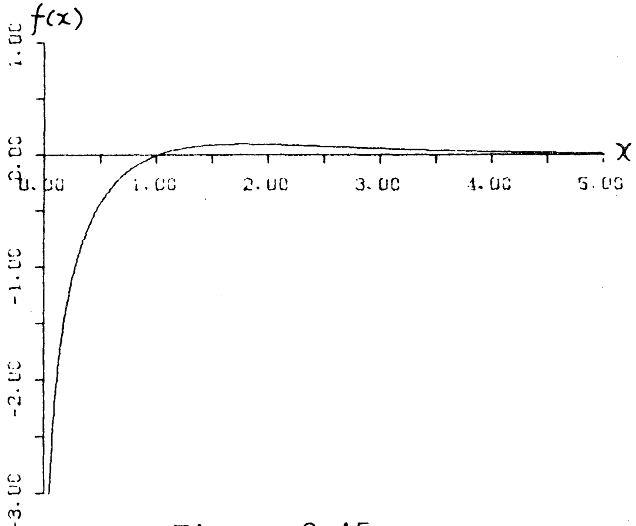



Figure 2-15

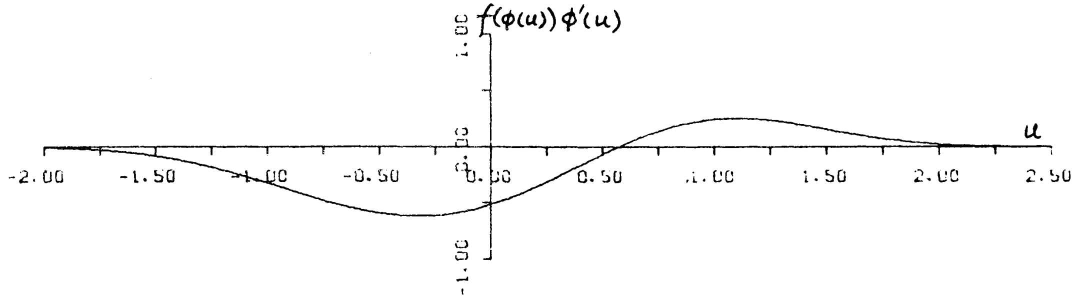



Figure 2-16

## 2.2 Choosing a quadrature formula

Table 2-1 supports the following statements:

i) For integrals over finite intervals, if the integrand has no singularity through the interval, CADRE or QUAD gets an advantage over DE (P2, P5, P7).

ii) For improper ingegrals over finite intervals with singularities at the endpoints of the interval, DE gets the best advantage and IMT gets the second best (P1, P4, P11).

iii) For integrals over infinite and semi-infinite intervals, if the integrand is not regular at infinity, DE is better than all the other formulas (e.g., $\int_0^\infty \exp(-x)\cdot\log x \, dx$). However, if the integrand is regular at infinity, it can be reduced to the case i) by suitable change of variable (e.g., $\int_0^\infty \frac{1}{1+x^4}dx = \int_0^{\frac{\pi}{2}} \frac{\cos^2\theta}{\cos^4\theta + \sin^4\theta} d\theta$ ). But even if DE may be used to evaluate the original integral, it will give slightly worse results than CADRE or QUAD.

iv) For integrals with singularity close to the real axis in the interior of the interval (e.g., K1), it is hard to evaluate the integral with desired accuracy using any of all the methods presented here, and DE is the most unsuccessful among them. But by splitting the integral into two integrals at the real part of the singular point, it can be reduced to case ii) .

## 3. Notes on usage of DE formula on digital computer.

Some notes must be necessary to effective use of DE formula.

### 3.1 A numerical technique by Takahashi and Mori to avoid subtractive cancellation by the factor $(1+x)^{\alpha}(1-x)^{\beta}$, $\alpha, \beta < 0$ .

In the case of integral $\int_{-1}^{1} f(x)\,dx$, $f(x)$ having a factor $(1+x)^{\alpha}(1-x)^{\beta}$, $\alpha,\beta<0$ (e.g., $f(x) = 1/\sqrt{1-x}$ , $1/\sqrt{\tan((\pi/2)\cdot(1+x))}$), the number of its significant digits decreases as $x \to \pm 1$ . Thus the relative error in the $f(x)$ will be greately increased. In such a case, following Takahashi and Mori [1] p.735, we must make the change of variable to avoid the cancellation; splitting the integral into two integrals, we have

$$(3.1\text{-}1) \qquad I = \int_{-1}^{1} f(x)\,dx = \int_{-1}^{0} f(x)\,dx + \int_{0}^{1} f(x)\,dx = I_1 + I_2$$

and we make direct substitution of $1 \pm x$ as follows:

$$(3.1\text{-}2) \qquad -t = 1+x = 1 + \tanh\left(\frac{\pi}{2}\sinh u\right) = \frac{\exp\left(\frac{\pi}{2}\sinh u\right)}{\cosh\left(\frac{\pi}{2}\sinh u\right)} \qquad t \in [-1,0]$$

$$(3.1\text{-}3) \qquad t = 1-x = 1 - \tanh\left(\frac{\pi}{2}\sinh u\right) = \frac{\exp\left(-\frac{\pi}{2}\sinh u\right)}{\cosh\left(\frac{\pi}{2}\sinh u\right)} \qquad t \in [0,1]$$

Then we obtain

$$(3.1\text{-}4) \qquad I_1 = \int_{-1}^{0} f(-1-t)\,dt = \int_{-\infty}^{0} f(-1-t(u)) \cdot \frac{\frac{\pi}{2}\cosh u}{\cosh^2\left(\frac{\pi}{2}\sinh u\right)}\,du$$

$$(3.1\text{-}5) \qquad I_2 = \int_{0}^{1} f(1-t)\,dt = \int_{0}^{\infty} f(1-t(u)) \cdot \frac{\frac{\pi}{2}\cosh u}{\cosh^2\left(\frac{\pi}{2}\sinh u\right)}\,du$$

3.2 Note on mechanizing DE formula on digital computer.

The essence of the technique described above is to substitute $\mp \exp(\pm\frac{\pi}{2}\sinh u) / \cosh(\frac{\pi}{2}\sinh u)$ directly into $t = \mp 1-x$ . Thus, it will be of no use to avoid cancellation to make the change of variable $x = -1-t$ for $x\in[-1,0]$ and $x = 1-t$ for $x\in[0,1]$ in library programs and to write $f(x)$ in its original form. Since the term $1+x$ will be evaluated not by $-t$ but by $1 + (-1-t)$, the loss of significance will be very large. Then we must transform $f(x)$ into the expression $g(t)$ of the independent variable $t = -1-x$ for $x\in[-1,0]$ , and $t = 1-x$ for $x\in[0,1]$. For example,

$$f(x) = (1+x)^{-\frac{1}{2}}(1-x)^{-\frac{1}{3}}$$

we must make transformation as follows:

$$f(x) = g(t) = \begin{cases} (-t)^{-\frac{1}{2}}(2+t)^{-\frac{1}{3}} & t\in[-1,0] \\ (2-t)^{-\frac{1}{2}}t^{-\frac{1}{3}} & t\in[0,1] \end{cases}$$

The same situation holds for the integral $\int_a^b f(x)dx$, if $f(x)$ has a factor $(x-a)^{\alpha}(b-x)^{\beta}$, $\alpha,\beta<0$ . In this case we must transform $f(x)$ into the expression of the variable $t = -\frac{2}{b-a}(x-a)$ for $x\in[a, \frac{a+b}{2}]$ and $t = \frac{2}{b-a}(b-x)$ for $x\in[\frac{a+b}{2}, b]$.

If this transformation is very tedious, we can transform the integral into an integral over $[0,\infty)$ by suitable change of variable (e.g., $x = \exp(-t)$), and then apply (2.1-2) or (2.1-3). For H1, by the change of variable $x = \exp(-t)$, we get

$$\text{H1'} \qquad I = \int_0^{\infty}\exp(-t)\log t\,dt$$

In this case, there is a problem how to choose the initial step size $h_0$ for H1. We shall consider this problem in the next section.

### 3.3 The initial step size $h_0$.

Our starting algorithm to find M, N such that $S_0 = \sum_{n=-M}^{N} f(\phi(nh_0))\cdot\phi'(nh_0)$, where $S_0$ is the first approximation of I, is as follows:

Input

$\varepsilon$ (some preassigned tolerance)

$h_0$ (initial step size)

Algorithm

```
h ← h0;   S0 ← f(φ(0))·φ'(0);   N ← 0;   M ← 0
for n=1,2,... do
    if N=0  then  Tn ← f(φ(nh))·φ'(nh)
                  if |Tn| ≤ |S0|*max(ε*10^-3, 10^-16)  then  N ← n
                                                       else  S0 ← S0 + Tn
                  endif
    endif
    if M=0  then  Un ← f(φ(-nh))·φ'(-nh)
                  if |Un| ≤ |S0|*max(ε*10^-3, 10^-16)  then  M ← n
                                                       else  S0 ← S0 + Un
                  endif
    endif
endfor
next:
```

Thus,

$$|T_n| \le |S_0| * \max(\varepsilon * 10^{-3}, 10^{-16}) \tag{3.3-1}$$
$$|U_n| \le |S_0| * \max(\varepsilon * 10^{-3}, 10^{-16})$$

must hold befor $nh_0$, $n=1,2,\ldots$, exceeds a certain threshold value which depends on representation of number by computer.

For example, in the case of H1, we have

$$I = \int_0^1 \log |\log x| dx = \int_{-1}^1 \frac{1}{2} \log \left|\log \frac{1+x}{2}\right| dx$$

$$= \int_{-1}^0 \frac{1}{2} \log \left|\log(-\frac{t}{2})\right| dt + \int_0^1 \frac{1}{2} \log \left|\log \frac{2-t}{2}\right| dt$$

where

$$-t = \frac{\exp(\frac{\pi}{2} \sinh u)}{\cosh(\frac{\pi}{2} \sinh u)} \qquad t \in [-1, 0]$$

$$t = \frac{\exp(-\frac{\pi}{2} \sinh u)}{\cosh(\frac{\pi}{2} \sinh u)} \qquad t \in [0, 1]$$

Since $2-t$ and $2$ are considered as the same values (additive no contribution) for $nh_0 > 3.45$ with double precision arithmetic in T-56, the second integrand $\frac{1}{2} \log \left|\log \frac{2-t}{2}\right|$ is regarded as $\log 0$ (error message "not allowed").

In the case of P7, we have

$$I = \int_0^1 \frac{x}{\exp x - 1} dx = \int_{-1}^1 \frac{1}{2} \cdot \frac{\frac{1+x}{2}}{\exp(\frac{1+x}{2}) - 1} dx$$

$$= \int_{-1}^0 \frac{1}{2} \cdot \frac{-\frac{t}{2}}{\exp(-\frac{t}{2}) - 1} dt + \int_0^1 \frac{1}{2} \cdot \frac{\frac{2-t}{2}}{\exp(\frac{2-t}{2}) - 1} dt$$

In the denominator of the first integral $\exp(-\frac{t}{2})$ is considered to be 1 for $nh_0 \geq 3.31$.

In both cases for large step size $h_0$, our starting algorithm results in failure by evaluating $f(\phi(nh_0)) \cdot \phi'(nh_0)$ or $f(\phi(-nh_0)) \cdot \phi'(-nh_0)$ at a point $nh_0$ beyond the limit 3.45 or 3.31 respectively. In contrast, it can be expected that by taking $h_0$ small enough depending on the tolerance $\varepsilon$ (3.3-1) can hold before $nh_0$ exceeds that threshold value. This is illustrated in Fig. 3.3-1.

```
ERROR REQUIREMENT      0.1000E-14     HO =  0.50000            P7 - 1

 FT957W ERROR AT(020531)    DIVIDE CHECK

 0.50000                 7                  7  0.7774990274260581
 0.25000                13                 13  0.7775046341101479      0.7211E-05
 0.12500                26                 26  0.7775046341122483      0.2701E-11

 S =  0.7775046341122483         ER =  0.1314E-16

 ERROR REQUIREMENT      0.1000E-14     HO =  0.25000           P7 - 2

  0.25000                13                 13  0.7775046341101479
  0.12500                26                 26  0.7775046341122483      0.2701E-11

 S =  0.7775046341122483          ER =  0.1358E-16


ERROR REQUIREMENT      0.1000E-11     HO =  0.50000            H1 - 1

 FT911W ERROR AT(020621)   DLOG    ARG= 0.0          ( ARG.LE.0 )          RESULT=(MIN VALUE)
 FT911W ERROR AT(020621)   DLOG    ARG= 0.0          ( ARG.LE.0 )          RESULT=(MIN VALUE)
 0.50000                   8              7 -0.2026589570990376E+56

ERROR REQUIREMENT      0.1000E-11     HO =  0.25000            H1 - 2

 0.25000                13                13 -0.5772156649014750

S =-0.5772156649015324     ER = 0.9944E-13   TRUE VALUE -0.5772156649015328608       ERROR -0.8648E-15
```

Figure 3.3-1

## 3.4 On the criterion of convergence.

Since the error term for DE formula with mesh size $h$ is roughly estimated (Ref. [5] p.265)

$$(3.4\text{-}1) \qquad |\Delta I_h| \simeq \exp(-\frac{A}{h})$$

where $A$ is a constant, we have

$$(3.4\text{-}2) \qquad |\Delta I_{\frac{h}{2}}| \simeq |\Delta I_h|^2$$

So that if we halve the mesh size, then the number of significant digits are doubled. Thus we can usually get the desired accuracy when

$$(3.4\text{-}3) \qquad |S_{i+1} - S_i| \leq \sqrt{\varepsilon}\,|S_{i+1}|$$

holds, except in the case where the integrand oscillates (e.g., P8 and P10).

In the above-mentioned case, however, on the safe side, we should like to test whether both

$$|S_{i+1} - S_i| \leq \varepsilon\,|S_{i+1}|$$

and

$$|S_{i+2} - S_{i+1}| \leq \varepsilon\,|S_{i+2}|$$

hold as the criteria of convergence. From Fig. 3.4-1, we see that (3.4-2) does not hold untill mesh size $h$ becomes small enough.

P6

ERROR REQUIREMENT 0.1000E-14 HO = 0.50000

| | | | | |
|---|---|---|---|---|
| 0.50000 | 7 | 7 | 1.145065201836647 | |
| 0.25000 | 13 | 13 | 1.109398079973005 | 0.3215E-01 |
| 0.12500 | 26 | 26 | 1.101740303515750 | 0.6951E-02 |
| 0.62500E-01 | 52 | 52 | 1.157349192484848 | 0.4805E-01 |
| 0.31250E-01 | 103 | 103 | 1.154711000023246 | 0.2285E-02 |
| 0.15625E-01 | 205 | 205 | 1.154700538516411 | 0.9060E-05 |
| 0.78125E-02 | 409 | 409 | 1.154700538379251 | 0.1188E-09 |

S = 1.154700538379251 ER = 0.7079E-17 TRUE VALUE 1.154700538379251529 ERROR -0.5033E-16

P8

ERROR REQUIREMENT 0.1000E-14 HO = 0.50000

| | | | | |
|---|---|---|---|---|
| 0.50000 | 6 | 6 | 0.2455391953890915 | |
| 0.25000 | 11 | 11 | 0.2312281657296014 | 0.6189E-01 |
| 0.12500 | 22 | 22 | 0.1126117247672289 | 0.1053E+01 |
| 0.62500E-01 | 44 | 44 | 0.6130785022273157E-01 | 0.8368E+00 |
| 0.31250E-01 | 87 | 88 | 0.3891818870620057E-01 | 0.5753E+00 |
| 0.15625E-01 | 173 | 175 | 0.9098637539166843E-02 | 0.3277E+01 |

S = 0.9098637539166843E-02 ER = 0.3978E-16

P10

ERROR REQUIREMENT 0.1000E-14 HO = 0.50000

| | | | | |
|---|---|---|---|---|
| 0.50000 | 7 | 7 | 1.873635947230349 | |
| 0.25000 | 14 | 14 | 0.8168465615955236 | 0.1294E+01 |
| 0.12500 | 27 | 27 | 0.8396163176771946 | 0.2712E-01 |
| 0.62500E-01 | 53 | 53 | 0.8386763427025238 | 0.1121E-02 |
| 0.31250E-01 | 105 | 105 | 0.8386763426944296 | 0.9651E-11 |

S = 0.8386763426944296 ER = 0.3249E-17

Figure 3.4-1

## 4. Difficult problems of integration

### 4.1 The restriction imposed by the number of bits for exponent.

The number of bits for exponent is usually taken to be 7 or 8 . Then, for example, the integral to get the abscissas of IMT formula

$$I = \int_0^t \exp(-\frac{1}{x} - \frac{1}{1-x})\, dx$$

$$= t\int_0^\infty \exp(-\frac{1}{t\,\exp(-x)})\, \exp(-\frac{1}{1-\,t\,\exp(-x)})\, \exp(-x)dx$$

with $t = 3/512,\ 2/512,\ 1/512$, has the value far smaller than $10^{-58}$. Thus, if we wish to evaluate this integral using DE formula (2.1-3), our algorithm will fail, since (3.3-1) is not satisfied before $nh=5.5$, with this $nh$ $x = \exp(nh-\exp(-nh))$ becomes 243.7 and $\exp(-x)$ vanishes.

Such a problem requires the use of multiple-precision arithmetic [6] .

## 5. Conclusion

We conclude from the experiment described above that DE formulas offer a very powerful method for numerical integration, except for the special cases described in the previous section. It is recommended to use DE formulas especially for integrals over infinite or semi-infinite intervals.

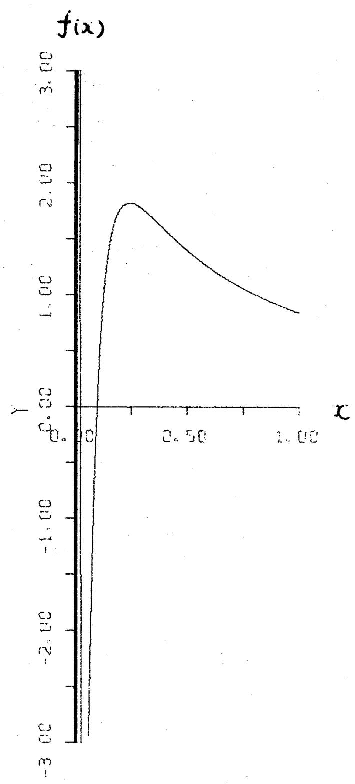
Appendix.

Dr. Rabinowitz presented the following problem when he visited ETL at Tsukuba on June 4,1980.

$$I = \int_0^1 f(x)dx = \int_0^1 \frac{\sin \frac{1}{\sqrt{x}}}{\sqrt{x}} dx \doteqdot 1.00813\ 41238\ 139$$

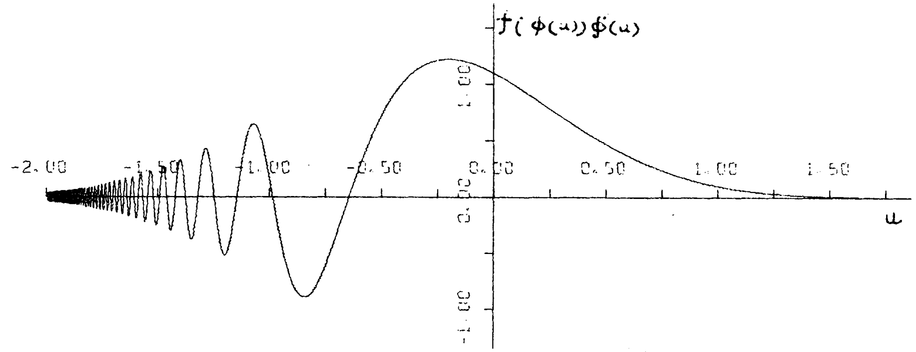
at x=0 value=0

We will show the results obtained by DE formulas below.



$$I = \int_{-1}^{0} \frac{\frac{1}{2}\sin\frac{1}{\sqrt{-t/2}}}{\sqrt{-t/2}}\,dt + \int_{0}^{1} \frac{\frac{1}{2}\sin\left(\frac{1}{\sqrt{(2-t)/2}}\right)}{\sqrt{(2-t)/2}}\,dt$$

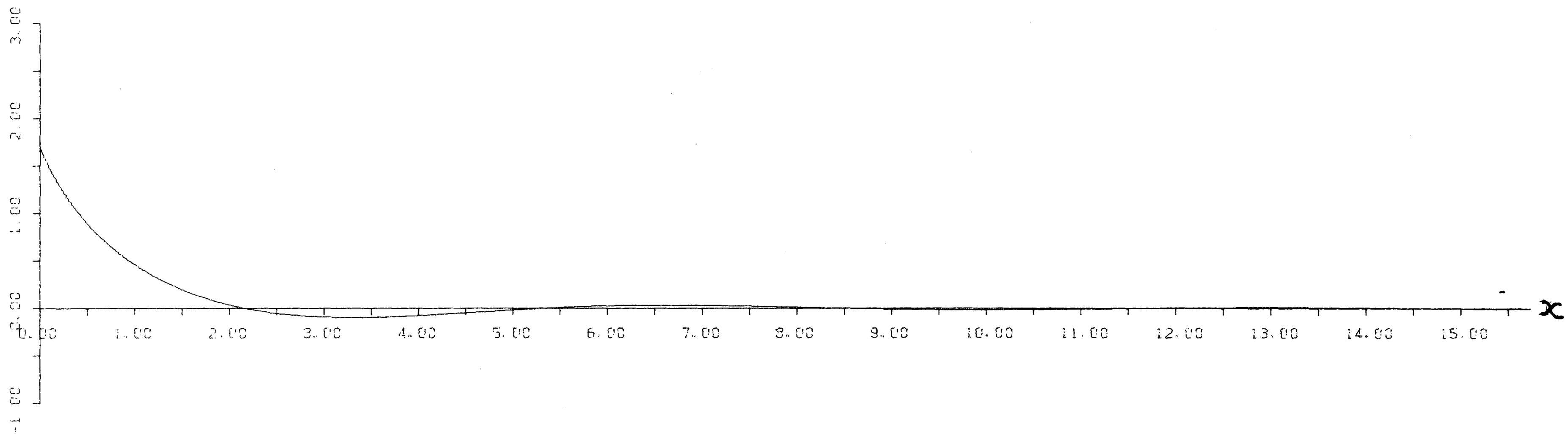
42



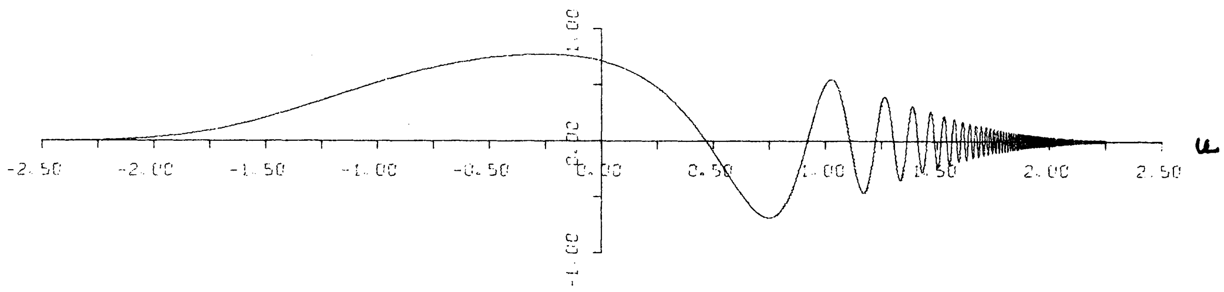

```
LIST 10@@0170-0270

0170       DOUBLE PRECISION FUNCTION FM1P11(X)
0180       DOUBLE PRECISION X, T, G
0190       IF(X) 1,2,2
0200 1      T = -0.5D0*X
0210       GO TO 3
0220 2      T = 1.0D0 - 0.5*X
0230  3      CONTINUE
0240       G = DSIN(1.0D0/DSQRT(T)) /DSQRT(T)
0250       FM1P11 = G / 2.0D0
0260       RETURN
0270       END

*RUN

PLEASE TYPE IN H0, EPS, LIST
=                   0.125D0                        1.0D-9   1
 0.12500              23          28   0.99630334357841 73
 0.62500E-01          46          56   0.981253506012 5632      0.1534E-01
 0.31250E-01          91         112    1.008041952064974       0.2657E-01
 0.15625E-01         181         224    1.003388731021478       0.4638E-02
 0.78125E-02         361         447    1.005907923892132       0.2504E-02
 0.39063E-02         721         893    1.008449386893941       0.2520E-02
 0.19531E-02        1441        1785    1.007959610813495       0.4859E-03
 0.97656E-03        2881        3569    1.008295296649887       0.3329E-03
 0.48828E-03        5761        7137    1.008103976816533       0.1898E-03
 0.24414E-03       11521       14273    1.008165123910790       0.6065E-04
 0.12207E-03       23041       28545    1.008143849296904       0.2110E-04
 0.61035E-04       46081       57089    1.008135239122684       0.8541E-05
 0.30518E-04       92161      114177    1.008135329025766       0.8918E-07
 0.15259E-04      184321      228353    1.008134649610200       0.6739E-06
 0.76294E-05      368641      456705    1.008134257201770       0.3892E-06
 0.38147E-05      737281      913409    1.008134050475504       0.2051E-06
 0.19073E-05     1474561     1826817    1.008134144078395       0.9285E-07
 0.95367E-06     2949121     3653633    1.008134131626789       0.1235E-07
*
                                                 ?
```

$$I = \int_0^1 \frac{\sin\left(\frac{1}{\sqrt{x}}\right)}{\sqrt{x}}\,dx = \int_0^\infty \frac{2\sin(1+x)}{(1+x)^2}\,dx \qquad \text{( by Dr. Rabinowitz's comment )}$$

$$f(x) = \frac{2\sin(1+x)}{(1+x)^2}$$




$f(\phi(u))\phi'(u)$

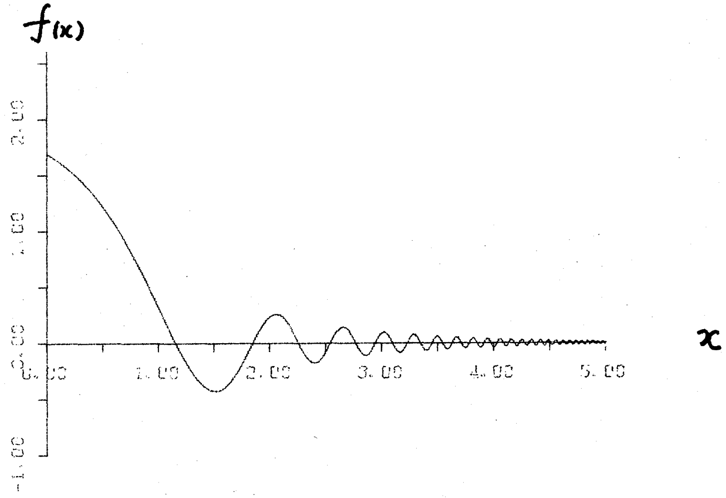


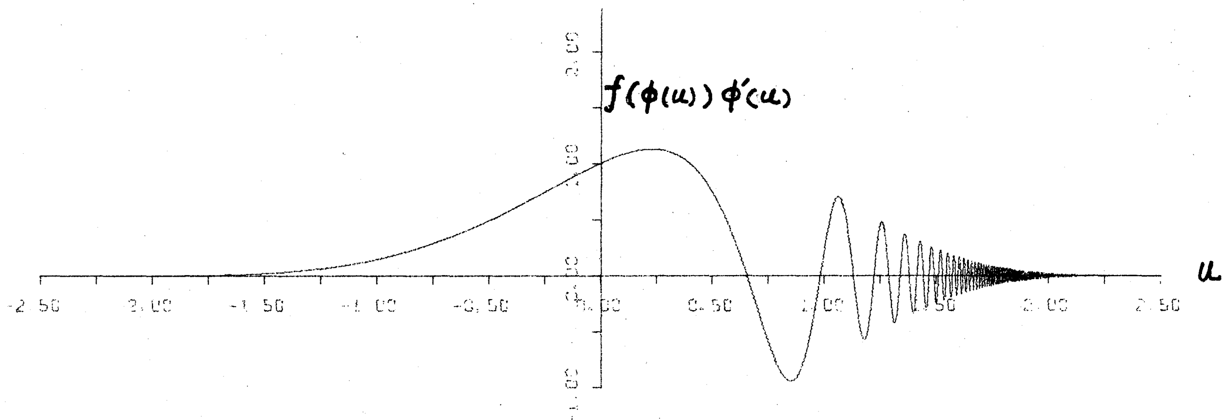
```
      LIST 180-1000

180         DOUBLE PRECISION FUNCTION F0INF(X)
190         DOUBLE PRECISION X
200          F0INF = 2.0D0*DSIN(1.0D0+X)/(1.0D0+X)**2
210         RETURN
220         END
```

$$I = 2\int_0^\infty \frac{\sin(1+x)}{(1+x)^2}\,dx$$

```
*RUN

            (C)  INTEGRATE(F0INF, 0, INF)

PLEASE TYPE IN  H0, EPS, LIST
=               0.03125D0                   1.0D-7   1
 0.31250E-01          100          105   1.000068727537460
 0.15625E-01          200          210   1.007688400674151     0.7562E-02
 0.78125E-02          400          419   1.006775973599763     0.9063E-03
 0.39063E-02          800          837   1.007513512037899     0.7320E-03
 0.19531E-02         1600         1673   1.007897695988269     0.3812E-03
 0.97656E-03         3199         3345   1.008203125717950     0.3029E-03
 0.48828E-03         6397         6689   1.008180234159500     0.2271E-04
 0.24414E-03        12793        13377   1.008170029883467     0.1012E-04
 0.12207E-03        25585        26753   1.008137971140978     0.3180E-04
 0.61035E-04        51169        53505   1.008139021682263     0.1042E-05
 0.30518E-04       102337       107009   1.008135015685097     0.3974E-05
 0.15259E-04       204673       214017   1.008133892035357     0.1115E-05
 0.76294E-05       409345       428033   1.008134156187340     0.2620E-06
 0.38147E-05       818689       856065   1.008134129054916     0.2691E-07

   1.008134129054916       0.2691E-07
                        ?
```

$$I = \int_0^1 \frac{\sin\left(\frac{1}{\sqrt{x}}\right)}{\sqrt{x}}\,dx = \int_0^\infty 2\,e^{-x}\sin(e^x)\,dx \equiv \int_0^\infty f(x)\,dx$$



$$I=\int_0^\infty 2\, e^{-x} \sin(e^{x})\, dx$$

```
 LIST 180-10000

180        DOUBLE PRECISION FUNCTION FEXP(X)
190         DOUBLE PRECISION X, DEXPF
200       FEXP= 2.0D0*DEXP(-X)*DSIN(DEXP(X))
210        RETURN
220        END


*RUN

          (D) INTEGRATE(FEXP, 0, INF)

PLEASE TYPE IN  H0, EPS, LIST
=                 0.125D0                   1.0D-9   1
 0.12500               27          26    1.071704042186671
 0.62500E-01           54          51    1.004933608340182     0.6644E-01
 0.31250E-01          107         101   0.996979779721295 0    0.7978E-02
 0.15625E-01          213         201    1.015120956996488     0.1787E-01
 0.78125E-02          425         401    1.009720373317079     0.5349E-02
 0.39063E-02          849         801    1.007896100079553     0.1810E-02
 0.19531E-02         1697        1601    1.008593032756302     0.6910E-03
 0.97656E-03         3393        3201    1.008131668867897     0.4576E-03
 0.48828E-03         6785        6401    1.008111677324365     0.1983E-04
 0.24414E-03        13569       12801    1.008157314514286     0.4527E-04
 0.12207E-03        27137       25601    1.008136230970505     0.2091E-04
 0.61035E-04        54273       51201    1.008135523133097     0.7021E-06
 0.30518E-04       108545      102401    1.008132923350206     0.2579E-05
 0.15259E-04       217089      204801    1.008134416324451     0.1481E-05
 0.76294E-05       434177      409601    1.008133909877286     0.5024E-06
 0.38147E-05       868353      819201    1.008134085382540     0.1741E-06
 0.19073E-05      1736705     1638401    1.008134103770320     0.1824E-07
 0.95367E-06      3473409     3276801    1.008134109726709     0.5908E-08
*                                                   ?
↑
BREAK
```

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